2-Bromo-1,1-dichloroethylene 5870-61-1 | DTXSID50207401

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 13.1 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.01e-01

Confidence level: 6.64e-01

Nearest Neighbors from the Training Set

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Methamidophos Measured: 2.68 Predicted: 6.06e-05 Image not found

2-Chlorobutane Measured: 69.0 Predicted: 117 Image not found

2,3-Dimethylbutane Measured: 4.62 Predicted: 313

Image not found

Pentatriacontane Measured: 12.0 Predicted: 8.42e-12 Image not found

Isopropanol
Measured: 197
Predicted: 23.4